```
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DICTIONARY FILE UPDATES:  10 APR 2007  HIGHEST RN 929680-66-0

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FILE LAST UPDATED: 10 Apr 2007  (20070410/ED)

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=> d stat que L31
L26          274 SEA FILE=CAPLUS ABB=ON  PLU=ON  ZARD S?/AU
L27           16 SEA FILE=CAPLUS ABB=ON  PLU=ON  GAGOSZ F?/AU
L28           73 SEA FILE=CAPLUS ABB=ON  PLU=ON  TOURNIER L?/AU
L29           10 SEA FILE=CAPLUS ABB=ON  PLU=ON  L26 AND (L27 OR L28)
L30            0 SEA FILE=CAPLUS ABB=ON  PLU=ON  L27 AND L28
L31           10 SEA FILE=CAPLUS ABB=ON  PLU=ON  (L29 OR L30)
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=> d stat que L32
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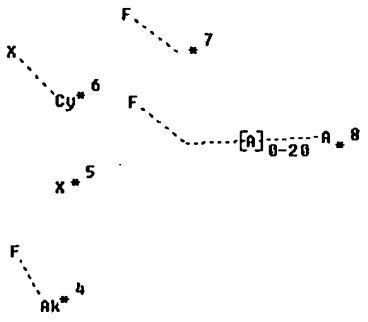
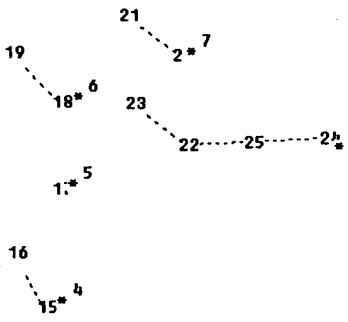
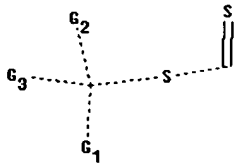
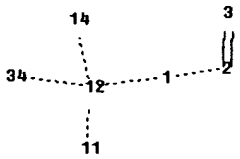
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

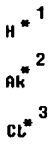
Structure attributes must be viewed using STN Express query preparation:
Uploading L10.str

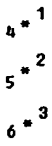












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3 4 5 6 11 15 16 17 18 19 20 21 23 34
ring/chain nodes :
1 2 12 14 22 24 25
chain bonds :
2-3 11-12 12-34 15-16 18-19 20-21 22-23
ring/chain bonds :
1-2 1-12 12-14 22-25 24-25
exact/norm bonds :
1-2 1-12 2-3 11-12 12-14 12-34 15-16 18-19 20-21 22-23 22-25 24-25

G1:[*1],[*2],[*3]

G2:O,S,Cl,Br,I,As,Sb,Se,Te

G3:[*4],[*5],[*6],[*7],[*8]

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:Atom 11:CLASS 12:CLASS 14:CLASS
15:CLASS 16:CLASS 17:CLASS 18:Atom 19:CLASS 20:CLASS 21:CLASS 22:CLASS
23:CLASS 24:CLASS
25:CLASS 34:CLASS
Generic attributes :
18:
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L15          22 SEA FILE=CAPLUS ABB=ON  PLU=ON  L12
L26         274 SEA FILE=CAPLUS ABB=ON  PLU=ON  ZARD S?/AU
L27          16 SEA FILE=CAPLUS ABB=ON  PLU=ON  GAGOSZ F?/AU
L28          73 SEA FILE=CAPLUS ABB=ON  PLU=ON  TOURNIER L?/AU
L32          10 SEA FILE=CAPLUS ABB=ON  PLU=ON  L15 AND (L26 OR L27 OR L28)

=> s L31-L32
L34          16 (L31 OR L32)

=> d ibib abs hitstr L34 1-16

L34  ANSWER 1 OF 16  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:        2006:847206  CAPLUS  Full-text
DOCUMENT NUMBER:         145:418930
TITLE:                   A flexible approach for the preparation of substituted
                         benzazepines: Application to the synthesis of
                         tolvaptan
AUTHOR(S):               Cordero-Vargas, Alejandro; Quiclet-Sire, Beatrice;
                         Zard, Samir Z.
CORPORATE SOURCE:        Laboratoire de Synthese Organique associe au CNRS,
                         Ecole Polytechnique, Palaiseau, 91128, Fr.
SOURCE:                  Bioorganic & Medicinal Chemistry (2006), 14(18),
                         6165-6173
                         CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER:               Elsevier B.V.
DOCUMENT TYPE:           Journal
LANGUAGE:                English
OTHER SOURCE(S):         CASREACT 145:418930
AB   A practical preparation of benzazepine derivs. using a series of radical and
     ionic reactions is reported.  This approach was applied to the synthesis of
     tolvaptan, a very promising vasopressin V2 receptor antagonist currently in
     clin. trials.
IT   517867-11-7P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of substituted benzazepines)
RN   517867-11-7  CAPLUS
CN   Propanoic acid, 2,2-dimethyl-, 1-[(ethoxythioxomethyl)thio]-4-(4-
     fluorophenyl)-4-oxobutyl ester (9CI)  (CA INDEX NAME)
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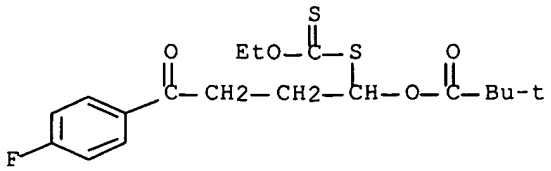


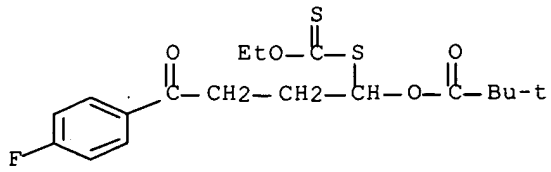
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:777862 CAPLUS Full-text
DOCUMENT NUMBER: 145:356139
TITLE: Radicals from aldehydes: a convergent access to dienes and δ-lactones
AUTHOR(S): Bagal, Sharanjeet K.; ***Tournier, Lucie***; ***Zard, Samir Z.***
CORPORATE SOURCE: Laboratoire de Synthese Organique associe au CNRS, Ecole Polytechnique, Palaiseau, 91128, Fr.
SOURCE: Synlett (2006), (10), 1485-1490
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:356139

AB A convenient method for the generation of O,S-acetal xanthates from aldehydes has been developed. The corresponding nucleophilic radicals undergo facile addition to unactivated olefins and the resulting adducts can be further elaborated to generate dienes and unsatd. δ-lactones. E.g., treating MeCHO with AcCl/ZnCl2, followed by EtOC(S)SK gave MeCH(Xa)OAc [Xa = SC(S)OEt]. Treating the latter with lauroyl peroxide and 1-octene gave 71% AcOCHMeCH2CH(Xa)C6H13.

IT ***517867-11-7P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(generation of O,S-acetal xanthates from aldehydes and their conversion to dienes and unsatd. δ-lactones)

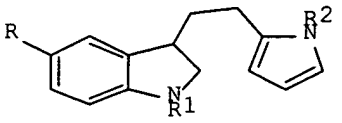
RN 517867-11-7 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 1-[(ethoxythioxomethyl)thio]-4-(4-fluorophenyl)-4-oxobutyl ester (9CI) (CA INDEX NAME)



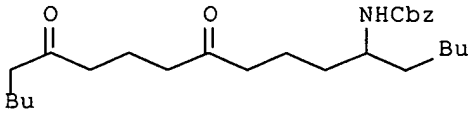
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:16004 CAPLUS Full-text
DOCUMENT NUMBER: 144:253791
TITLE: S-(3-Chloro-2-oxo-propyl)-O-ethyl xanthate: a linchpin radical coupling agent for the synthesis of heterocyclic and polycyclic compounds
AUTHOR(S): Bergeot, Olga; Corsi, Camilla; El Qacemi, Myriem; ***Zard, Samir Z.***
CORPORATE SOURCE: Laboratoire de Synthese Organique associe au CNRS, Ecole Polytechnique, Palaiseau, 91128, Fr.
SOURCE: Organic & Biomolecular Chemistry (2006), 4(2), 278-290
CODEN: OBCRAK; ISSN: 1477-0520
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:253791
GI



III



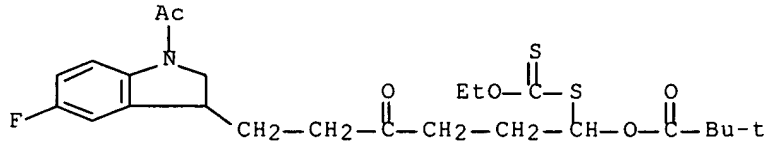
IV

AB 3-Chlorooxopropyl-O-Et xanthate ClCH2COCH2SC(:S)OEt (I) is prepared; radical-mediated addns. of I to alkenes yield α-(4-chloro-3- oxopropyl)xanthates which can be converted to a variety of compds. Reaction of 1,3-dichloroacetone and potassium O-Et xanthate in water yields I in good purity; use of acetone as solvent gives a mixture of I and the dixanthate EtOC(:S)SCH2COCH2SC(:S)OEt (no data) which gives lower yields of product in radical-mediated addition reactions than pure I. Dilauryl peroxide-mediated addition of I to alkenes such as N-arylallylamine derivs. 4-RC6H4N(R1)CH2CH:CH2 (R = MeO, Cl, Br, F; R1 = MeSO2, MeCO) provides α-(4-chloro-3-oxobutyl)xanthates such as 4-RC6H4N(R1)CH2CH(SCO2Et)CH2CH2COCH2Cl (R = MeO, Cl, Br, F; R1 = MeSO2, MeCO; II) in 35-89% yields. II (R = MeO, Cl, Br, F; R1 = MeSO2, MeCO) are converted to the readily oxidized pyrrolylethylindolines III (R = MeO, Cl, Br, F; R1 = MeSO2, MeCO; R2 = H, cyclopropyl, cyclohexyl, 4-MeOC6H4CH2) by radical mediated cyclization followed by substitution of the chloro group with potassium ethylxanthate, radical-mediated addition of the xanthate to vinyl pivaloate with concurrent xanthate migration, and treatment with amines R2NH2 (R2 = H, cyclopropyl, cyclohexyl, 4-MeOC6H4CH2); related thiazolylethylindolines are prepared by reaction of a chlorooxobutylindoline intermediate with either N-acetylthiourea or 3-pyridinecarbothioamide. Using I, dioxononadecanylcarbamate IV, a potential precursor for perhydrohistrionicotoxin, is prepared in seven steps with a longest linear sequence of six steps; efforts to convert IV to perhydrohistrionicotoxin have not been successful.
IT ***877082-63-8P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrrolylethylindolines using the preparation of α-(4-chloro-3-oxobutyl) O-Et xanthates by radical-mediated coupling reactions of alkenes with S-(3-chloro-2-oxopropyl)-O-Et xanthate as the key step)

RN 877082-63-8 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 6-(1-acetyl-5-fluoro-2,3-dihydro-1H-indol-3-yl)-1-[(ethoxythioxomethyl)thio]-4-oxohexyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:982358 CAPLUS Full-text

DOCUMENT NUMBER: 143:266831

TITLE: Improved process for the preparation of benzazepines and their derivatives

INVENTOR(S): ***Zard, Samir***; Cordero Vargas, Alejandro; Sire, Beatrice

PATENT ASSIGNEE(S): Centre National de la Recherche Scientifique CNRS, Fr.; Ecole Polytechnique

SOURCE: Fr. Demande, 54 pp.
CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2867187	A1	20050909	FR 2004-50416	20040302
CA 2557731	A1	20050915	CA 2005-2557731	20050221
WO 2005085183	A1	20050915	WO 2005-FR50110	20050221
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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1720827	A1	20061115	EP 2005-728103	20050221
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				

PRIORITY APPLN. INFO.: FR 2004-50416 A 20040302
WO 2005-FR50110 W 20050221

OTHER SOURCE(S): CASREACT 143:266831; MARPAT 143:266831

GI

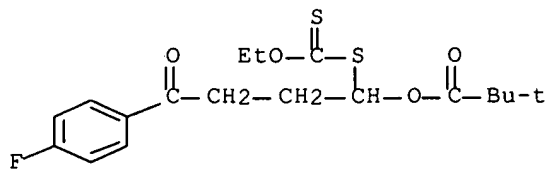
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention is related to a process for the preparation of benzazepines I [R1 = independently halo, aryl/halo/alkyl, acyl, OH and derivs., etc.; n = 0-4; when n ≥ 2, R1s can form a hydrocarbon cycle or heterocycle; R2-R7 = independently H, halo, halogenoalkyl, heterocyclyl, aryl, etc.; or one or more pairs of R4-R7 form one or more hydrocarbon cycle(s) or heterocycle(s) with at least one of R4-R7 = H] by (a) radical addition of olefins of formula R7R6C:CR4R5 [R4-R7 = defined as above] to compds. II [Z1 = halogeno/alkoxy, alkyl, acyl, etc.; R2a = H, halo, halogeno/alkyl, aryl, acyl, etc.; R1, n = defined as above] e.g. xanthates; (b) radical cyclization of III [R1, R2a, R4-R7, Z1, n = defined as above]; (c) oximation of tetralones IV [R1, R2a, R4-R7, Z1, n = defined as above]; (d) Beckmann rearrangement of the oximes and reduction(s) without isolation of the intermediate(s). The advantages include higher product yields, absence of drastic conditions, and preparation of functionalized benzazepines. Thus, reacting S-[2-(4-Chlorophenyl)-2-oxoethyl] O-Et dithiocarbonate (preparation given) with vinyl pivalate in DCM, followed by cyclization, and oximation of the tetralone intermediate gave oxime (E)-V. Rearrangement of oxime (E)-V in DCM in the presence of PCl5 and double reduction with Zn/AcOH, and BH3•THF in THF gave benzazepine VI (no isolation of the intermediates).

IT ***517867-11-7P***, 1-(Ethoxythiocarbonylsulfanyl)-4-(4-fluorophenyl)-4-oxobutyl 2,2-Dimethylpropionate
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of benzazepines by homolytic addition of olefins to xanthates, radical cyclization, oximation of tetralones, and Beckmann rearrangement/reduction(s))

RN 517867-11-7 CAPLUS

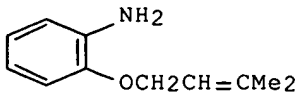
CN Propanoic acid, 2,2-dimethyl-, 1-[(ethoxythioxomethyl)thio]-4-(4-fluorophenyl)-4-oxobutyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:44329 CAPLUS Full-text
DOCUMENT NUMBER: 142:261339
TITLE: A practical variation on the Leuckart reaction
AUTHOR(S): ***Tournier, Lucie; Zard, Samir Z.***
CORPORATE SOURCE: Laboratoire de Synthese Organique associe au CNRS, Ecole Polytechnique, Palaiseau, F-91128, Fr.

SOURCE: Tetrahedron Letters (2005), 46(6), 971-973
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:261339
GI



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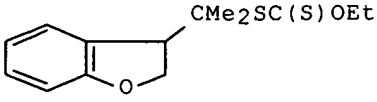


II

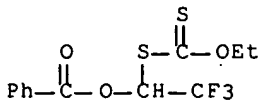
AB S-Aryldiazo xanthates, derived from the corresponding diazonium salts by reaction with potassium O-Et xanthate, undergo a radical chain reaction with loss of nitrogen; the intermediate aromatic radical can be captured by an internal olefin to give bicyclic xanthates in good overall yield. E.g., diazotization of O-prenylated 2-aminophenol I was followed by addition of cyclohexane and the medium deoxygenated by bubbling nitrogen to avoid interference by triplet oxygen. Potassium O-Et xanthate was then incorporated to result in dihydrobenzofuran II.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

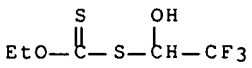
L34 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1155996 CAPLUS Full-text
DOCUMENT NUMBER: 142:239838
TITLE: A direct approach to α-hydroxy and α-chloro trifluoromethyl derivatives
AUTHOR(S): ***Tournier, Lucie; Zard, Samir Z.***
CORPORATE SOURCE: Laboratoire de Synthese Organique associe au CNRS, Ecole Polytechnique, Palaiseau, 91128, Fr.
SOURCE: Tetrahedron Letters (2005), 46(3), 455-459
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:239838

AB S-1-Acyloxy-2,2,2-trifluoroethyl and S-1-chloro-2,2,2-trifluoroethyl dithiocarbonates add efficiently to various functionalised olefins to give the corresponding adducts via a radical chain reaction initiated by a small amount of lauroyl peroxide.

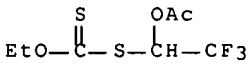
IT ***845523-74-2***
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of α-hydroxy and α-chloro trifluoromethyl derivs.)
RN 845523-74-2 CAPLUS
CN Carbonodithioic acid, S-[1-(benzoyloxy)-2,2,2-trifluoroethyl] O-ethyl ester (9CI) (CA INDEX NAME)



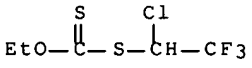
IT *845523-49-1P 845523-51-5P 845523-76-4P*
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of α-hydroxy and α-chloro trifluoromethyl derivs.)
RN 845523-49-1 CAPLUS
CN Carbonodithioic acid, O-ethyl S-(2,2,2-trifluoro-1-hydroxyethyl) ester (9CI) (CA INDEX NAME)



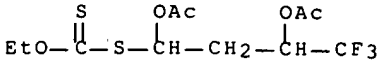
RN 845523-51-5 CAPLUS
CN Carbonodithioic acid, S-[1-(acetyloxy)-2,2,2-trifluoroethyl] O-ethyl ester (9CI) (CA INDEX NAME)



RN 845523-76-4 CAPLUS
CN Carbonodithioic acid, S-(1-chloro-2,2,2-trifluoroethyl) O-ethyl ester (9CI) (CA INDEX NAME)



IT *845523-54-8P*
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of α-hydroxy and α-chloro trifluoromethyl derivs.)
RN 845523-54-8 CAPLUS
CN Carbonodithioic acid, S-[1,3-bis(acetyloxy)-4,4,4-trifluorobutyl] O-ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:203169 CAPLUS Full-text
DOCUMENT NUMBER: 140:253264
TITLE: Preparation of thiocarbonylsulfanyl derivatives for radical synthesis of alpha-perfluoroalkylamine compounds by dimerization and by their addition to olefins
INVENTOR(S): ***Zard, Samir; Gagosz, Fabien***
PATENT ASSIGNEE(S): Rhodia Chimie, Fr.
SOURCE: Fr. Demande, 71 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2844264	A1	20040312	FR 2002-11261	20020911
FR 2844264	B1	20061020		
WO 2004024681	A2	20040325	WO 2003-FR2697	20030911
WO 2004024681	A3	20040701		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003276330	A1	20040430	AU 2003-276330	20030911
EP 1539688	A2	20050615	EP 2003-795042	20030911
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1688541	A	20051026	CN 2003-824457	20030911
JP 2005538174	T	20051215	JP 2004-535602	20030911
US 2006122404	A1	20060608	US 2005-527702	20050311

PRIORITY APPLN. INFO.:
FR 2002-11261 A 20020911
WO 2003-FR2697 W 20030911

OTHER SOURCE(S): MARPAT 140:253264
GI

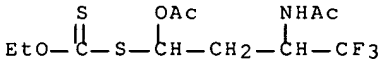
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention is directed to the preparation of I and their use in radical synthesis of α-perfluoroalkylamines [wherein Z1 = alk(en/yn)yl, acyl, aryl, aralkyl, cyclohydrocarbyl, heterocyclyl, etc.; Z2, Z3 = independently H, cyclo/alkyl, aryl, electron-withdrawing group, with the proviso that Z2 and Z3 induce an electron-withdrawing effect with respect to the nitrogen they are bound; Z4 = H, cyclo/alkyl; R = halo, in particular F]. Specifically, II were prepared by radical addition of I to an olefin Z5Z7C:CZ6Z8 and III by radical dimerization of I [wherein R, Z1, Z2, Z3, Z4 are defined as above; Z5, Z6, Z7,

Z8 = independently H, halo, halogeno/alkyl, aryl/alkenyl, aryl/alkynyl, acyl, aryl, cyclohydrocarbyl, heterocyclyl, polymeric chain, etc.]. The advantages include a direct, and efficient method with high yields, minimization of number of steps, and mild reaction conditions. For example, IV was prepared by nucleophilic substitution of 2,2,2-trifluoro-1-methoxyethanol, halogenation of the alc., N-(2,2,2-trifluoro-1-hydroxyethyl)acetamide, followed by substitution of the chloro intermediate with potassium ethylxanthogenate. V was prepared by radical addition of allyl acetate to IV in the presence of 1,2-dichloroethane and DLP. Simillarly, VI was prepared by radical dimerization of IV in the presence of chlorobenzene and DLP., and separated into its two diastereomers.

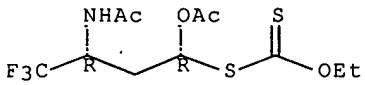
IT ***583028-99-3P 669692-45-9P***
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(α-trifluoromethylacetylamino product; preparation of thiocarbonylsulfanyl derivs. for radical synthesis of alpha-perfluoroalkylamine compds. by addition to olefins and dimerization)

RN 583028-99-3 CAPLUS
CN Carbonodithioic acid, S-[3-(acetylamino)-1-(acetyloxy)-4,4,4-trifluorobutyl] O-ethyl ester (9CI) (CA INDEX NAME)



RN 669692-45-9 CAPLUS
CN Carbonodithioic acid, S-[(1R,3R)-3-(acetylamino)-1-(acetyloxy)-4,4,4-trifluorobutyl] O-ethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:501664 CAPLUS Full-text
DOCUMENT NUMBER: 139:197168
TITLE: A Direct Approach to α-Trifluoromethylamines
AUTHOR(S): ***Gagosz, Fabien; Zard, Samir Z.***
CORPORATE SOURCE: Laboratoire de Synthese Organique associe, CNRS Ecole Polytechnique, Palaiseau, 91128, Fr.
SOURCE: Organic Letters (2003), 5(15), 2655-2657
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:197168

AB S-[1-(N-Acetylamino)-2,2,2-trifluoroethyl]-O-Et dithiocarbonate, a readily available xanthate, adds efficiently to various functionalized olefins CH2:CHR

[R = OAc, CH2CN, CH(OEt)2, etc.] to give the corresponding adducts F3CCH(NHAc)CH2CH(R)SC(S)OEt via a radical chain reaction initiated by a small amount of lauroyl peroxide.

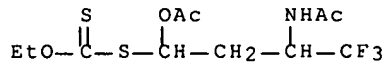
IT ***583028-99-3P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of (acetylamino)(ethoxythiocarbonylsulfanyl)trifluorobutyl esters by radical addition reaction of S-[1-(N-acetylamino)-2,2,2-trifluoroethyl]-O-Et dithiocarbonate to olefins)

RN 583028-99-3 CAPLUS

CN Carbonodithioic acid, S-[3-(acetylamino)-1-(acetyloxy)-4,4,4-trifluorobutyl] O-ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:415873 CAPLUS Full-text

DOCUMENT NUMBER: 139:292179

TITLE: A new, unexpected synthesis of 1,3-dithietanones

AUTHOR(S): Quiclet-Sire, Beatrice; Sanchez-Jimenez, Graciela; ***Zard, Samir Z.***

CORPORATE SOURCE: Laboratoire de Synthese Organique Associe au CNRS, Ecole Polytechnique, Palaiseau, 91128, Fr.

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2003), (12), 1408-1409
CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:292179

AB Treatment of a geminal pivaloxy xanthate, prepared by an intermol. radical addition of a xanthate to vinyl pivalate, gives a 1,3-dithietanone, a little known class of compds. The radical addition reaction of carbonodithioic acid O-Et S-(2-oxo-2-phenylethyl) ester with vinyl pivalate gave 2,2-dimethylpropanoic acid 1-[(ethoxythioxomethyl)thio]-4-oxo-4- phenylbutyl ester. The titanium chloride (TiCl4)-mediated reaction of the latter gave 4-(3-oxo-3-phenylpropyl)-1,3-dithietan-2-one. Heating the latter in 1,2-dichlorobenzene resulted in the formation of 2-phenylthiophene.

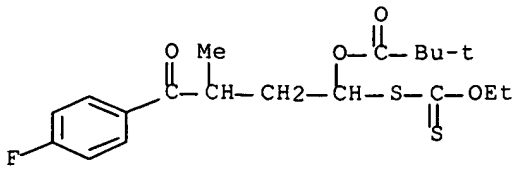
IT ***517867-28-6***

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of 1,3-dithietanones from dimethylpropanoic acid [(ethoxythioxomethyl)thio]oxoalkyl esters)

RN 517867-28-6 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 1-[(ethoxythioxomethyl)thio]-4-(4-fluorophenyl)-3-methyl-4-oxobutyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

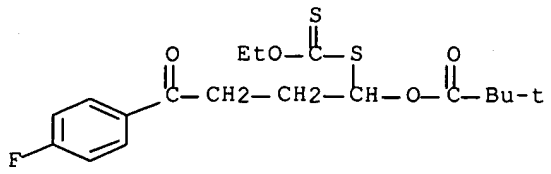
L34 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:155668 CAPLUS Full-text
DOCUMENT NUMBER: 139:53084
TITLE: A practical radical based access to functionalized geminal bisphosphonates
AUTHOR(S): ***Gagosz, Fabien; Zard, Samir Z.***
CORPORATE SOURCE: Laboratoire de Synthese Organique associe au CNRS, Ecole Polytechnique, Palaiseau, 91128, Fr.
SOURCE: Synlett (2003), (3), 387-389
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:53084
AB Xanthate derivs. of tetraalkylmethylenebisphosphonate, EtOC(S)SCH[P(O)(OR)2]2 (R = Me, Et) add efficiently to various functionalized olefins, e.g., CH2:CHR' (R' = CH2OAc, CH2CH2C(O)Me, CH2TMS, CH2CN, p-C6H4Cl, p-C6H4Br) to give the corresponding adducts, e.g., EtOC(S)SCHR'CH2CH[P(O)(OR)2]2, via a radical chain reaction initiated by a small amount of lauroyl peroxide.
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:54459 CAPLUS Full-text
DOCUMENT NUMBER: 138:337923
TITLE: A practical variation on the Paal-Knorr pyrrole synthesis
AUTHOR(S): Quiclet-Sire, Beatrice; Quintero, Leticia; Sanchez-Jimenez, Graciela; ***Zard, Samir Z.***
CORPORATE SOURCE: Laboratoire de Synthese Organique associe au CNRS, Ecole Polytechnique, Palaiseau, 91128, Fr.
SOURCE: Synlett (2003), (1), 75-78
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:337923
AB The radical addition of α-xanthyl ketones, e.g. O-ethyl-S-(4-fluorophenacyl)dithiocarbonate, to vinyl pivalate gives xanthate adducts, such as Et S-[1-tert-butylcarbonyloxy-(4-fluorophenacyl)ethyl] xanthate, which are synthetic equivalent of 1,4-keto aldehydes; treatment with ammonia or primary amines leads to the corresponding pyrroles, e.g. 2-(4-fluorophenyl)-1-benzylpyrrole, in high yield.
IT ***517867-11-7P 517867-28-6P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of pyrrole derivs. via radical addition of xanthyl ketones to vinyl pivalate and Paal-Knorr reaction with ammonia or primary amines)

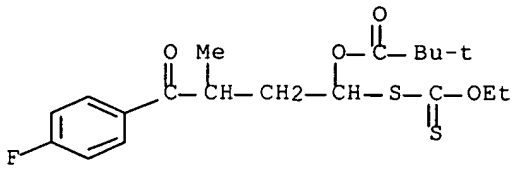
RN 517867-11-7 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 1-[(ethoxythioxomethyl)thio]-4-(4-fluorophenyl)-4-oxobutyl ester (9CI) (CA INDEX NAME)



RN 517867-28-6 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 1-[(ethoxythioxomethyl)thio]-4-(4-fluorophenyl)-3-methyl-4-oxobutyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:835073 CAPLUS Full-text

DOCUMENT NUMBER: 138:73217

TITLE: Tin-Free Radical Sequences under Acidic Conditions. Convergent Access to Azole-Containing Structures

AUTHOR(S): ***Gagosz, Fabien; Zard, Samir Z.***

CORPORATE SOURCE: Laboratoire de Synthese Organique associe au CNRS, Ecole Polytechnique, Palaiseau, 91128, Fr.

SOURCE: Organic Letters (2002), 4(24), 4345-4348
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:73217

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Xanthates such as I add efficiently to olefins bearing [1,2,4]triazole, imidazole, or benzimidazole moieties in the presence of camphorsulfonic acid via a radical chain reaction initiated by a small amount of lauroyl peroxide

to provide saturated xanthates such as II in 61-88% yields. The use of an acidic and anhydrous medium inhibits nucleophilic attack of the basic heterocycles at the xanthate moiety and allows radical reactions to occur. Xanthates II undergo cyclization to give fused heterocycles including a tetralone, a benzazepinone, and pyrroloimidazole III in 36-75% yields. Fused heteroarom. compds. are also prepared directly from azole-containing alkenes and xanthates such as I by a tandem radical addition/cyclization to provide pyrrolobenzimidazoles such as IV with structural similarity to known anticancer agents. Nucleophilic substitution of IV with amines and a benzyl alc. provides carboxylic acid ester and amide derivs. of IV in 85-91% yields.

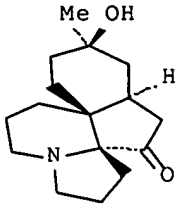
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:509567 CAPLUS Full-text
DOCUMENT NUMBER: 137:216832
TITLE: A New Tin-Free Source of Amidyl Radicals
AUTHOR(S): ***Gagosz, Fabien***; Moutrille, Cecile; ***Zard, Samir Z.***
CORPORATE SOURCE: Laboratoire de Synthese Organique associe au CNRS, Ecole Polytechnique, Palaiseau, 91128, Fr.
SOURCE: Organic Letters (2002), 4(16), 2707-2709
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:216832

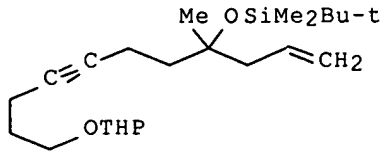
AB The readily available N-(O-Et thiocarbonylsulfanyl)amides are powerful amidyl radical precursors that undergo 5-exo cyclization to give pyrrolidinone derivs. via a radical-chain reaction initiated by a small amount of lauroyl peroxide.

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:418601 CAPLUS Full-text
DOCUMENT NUMBER: 137:201464
TITLE: A short synthesis of (±)-13-deoxyserratine
AUTHOR(S): Cassayre, Jerome; ***Gagosz, Fabien***; ***Zard, Samir Z.***
CORPORATE SOURCE: Syngenta, Basel, 4002, Switz.
SOURCE: Angewandte Chemie, International Edition (2002), 41(10), 1783-1785
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:201464
GI



I



II

AB A short and efficient total synthesis of (±)-13-deoxyserratine (I) features a highly stereoselective intramol. Pauson - Khand reaction of II and a cascade of radical cyclizations. The desired alkaloid I was thus obtained in ten steps in an overall yield of 12%.

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

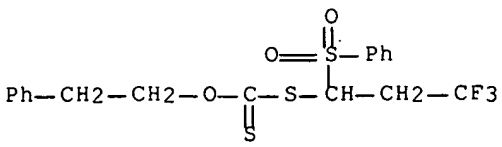
L34 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:174719 CAPLUS Full-text
DOCUMENT NUMBER: 134:353104
TITLE: A Xanthate Transfer Radical Process for the Introduction of the Trifluoromethyl Group
AUTHOR(S): Bertrand, Frederique; Pevere, Virginie; Quiclet-Sire, Beatrice; ***Zard, Samir Z.***
CORPORATE SOURCE: Institut de Chimie des Substances Naturelles, C.N.R.S., Gif-sur-Yvette, 91198, Fr.
SOURCE: Organic Letters (2001), 3(7), 1069-1071
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:353104

AB S-Trifluoromethyl xanthates efficiently add to unactivated alkenes by a radical mechanism to give adducts with a trifluoromethyl group at the least hindered terminus of the olefin.

IT ***339300-31-1P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(addition of trifluoromethyl radical to unactivated alkenes)

RN 339300-31-1 CAPLUS

CN Carbonodithioic acid, O-(2-phenylethyl) S-[3,3,3-trifluoro-1-(phenylsulfonyl)propyl] ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:800862 CAPLUS Full-text

DOCUMENT NUMBER: 132:151635
TITLE: Generation and capture of iminyl radicals from ketoxime xanthates
AUTHOR(S): ***Gagosz, Fabien; Zard, Samir Z.***
CORPORATE SOURCE: Institut Chimie Substances Naturelles, Gif-sur-Yvette, F-91198, Fr.
SOURCE: Synlett (1999), (12), 1978-1980
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:151635
AB Irradiation of ketoxime O-(S-Me xanthates) containing a γ,δ-double bound leads to a hydropyrrole through cyclization of an intermediate iminyl radical in a radical chain reaction. The last propagation step involves transfer of a dithiocarbonate group, and various external radical traps can be incorporated into the medium, allowing access to a variety of substituted dihydropyrroles.
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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DICTIONARY FILE UPDATES: 10 APR 2007 HIGHEST RN 929680-66-0

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FILE COVERS 1907 - 11 Apr 2007 VOL 146 ISS 16
FILE LAST UPDATED: 10 Apr 2007 (20070410/ED)

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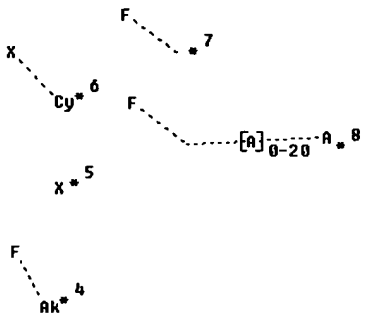
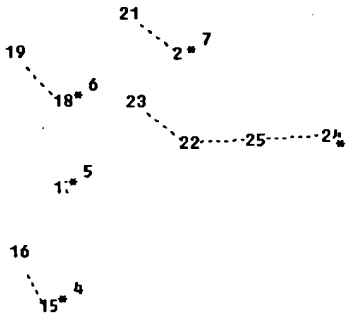
=> d stat que L15
L10 STR

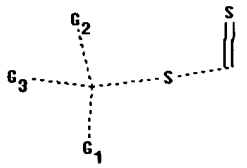
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

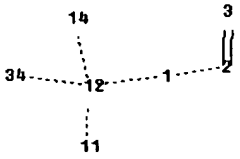
Structure attributes must be viewed using STN Express query preparation:

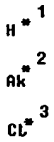
Uploading L10.str

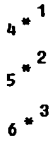












chain nodes :
3 4 5 6 11 15 16 17 18 19 20 21 23 34
ring/chain nodes :
1 2 12 14 22 24 25
chain bonds :
2-3 11-12 12-34 15-16 18-19 20-21 22-23
ring/chain bonds :
1-2 1-12 12-14 22-25 24-25
exact/norm bonds :
1-2 1-12 2-3 11-12 12-14 12-34 15-16 18-19 20-21 22-23 22-25 24-25

G1:[*1],[*2],[*3]

G2:O,S,Cl,Br,I,As,Sb,Se,Te

G3:[*4],[*5],[*6],[*7],[*8]

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:Atom 11:CLASS 12:CLASS 14:CLASS
15:CLASS 16:CLASS 17:CLASS 18:Atom 19:CLASS 20:CLASS 21:CLASS 22:CLASS
23:CLASS 24:CLASS
25:CLASS 34:CLASS
Generic attributes :
18:

Saturation : Unsaturated

L12 31 SEA FILE=REGISTRY SSS FUL L10
L15 22 SEA FILE=CAPLUS ABB=ON PLU=ON L12

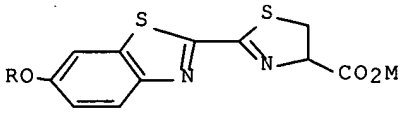
=> s l15 not L34
L35 12 L15 NOT L34

=> d ibib abs hitstr L35 1-12

L35 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:171575 CAPLUS Full-text
DOCUMENT NUMBER: 146:295906
TITLE: Preparation of firefly luciferin derivatives
INVENTOR(S): Lu, Linlin; Jin, Zhenhua; Dong, Bing
PATENT ASSIGNEE(S): Shenyang Zhongke Liangma Bioengineering Co., Ltd., Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 11pp. CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1911917	A	20070214	CN 2006-10047452	20060815

PRIORITY APPLN. INFO.: CN 2006-10047452 20060815
GI

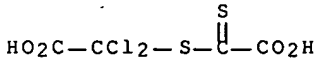


I

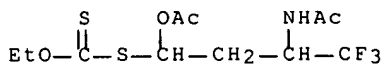
AB The title compds. I (R = H, alkyl, or acyl; and M = ammonium, sodium, potassium, or calcium), useful for food and vegetable anal., are prepared by alkali catalyzed cyclization of benzothiazolecarbonyl fluoride with D-cysteine.

IT ***928202-87-3P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of firefly luciferin derivs.)

RN 928202-87-3 CAPLUS
CN Acetic acid, 2-[(carboxythioxomethyl)thio]-2,2-dichloro- (CA INDEX NAME)



L35 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:358951 CAPLUS Full-text
Correction of: 2005:1110266
DOCUMENT NUMBER: 145:356107
Correction of: 143:346554
TITLE: Synthesis of amides with retention of the functional group
AUTHOR(S): Li, W.-R.
CORPORATE SOURCE: Germany
SOURCE: Science of Synthesis (2005), 21, 179-257
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review of the synthesis of amides with focus on processes that retain functional groups.
IT ***583028-99-3P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of amides)
RN 583028-99-3 CAPLUS
CN Carbonodithioic acid, S-[3-(acetylamino)-1-(acetyloxy)-4,4,4-trifluorobutyl] O-ethyl ester (9CI) (CA INDEX NAME)



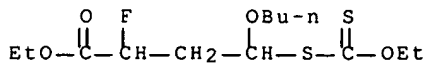
L35 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:165894 CAPLUS Full-text
DOCUMENT NUMBER: 144:412819
TITLE: Synthesis of 2,3-trans Di-Substituted Tetrahydrofurans through Sequential Xanthate Radical Addition-Substitution Reactions
AUTHOR(S): Jean-Baptiste, Laeetitia; Yemets, Sergiy; Legay, Remi; Lequeux, Thierry
CORPORATE SOURCE: Laboratoire de Chimie Moleculaire et Thioorganique, UMR CNRS 6507, ENSICAEN-Universite de Caen, Caen, F-14050, Fr.
SOURCE: Journal of Organic Chemistry (2006), 71(6), 2352-2359
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:412819
AB A two-step preparation of 2,3-trans disubstituted THF derivs. is reported from S-alkyl dithio-carbonates. The study of the group transfer reaction from xanthate and alkenes afforded intermediate S-alkyl dithio-carbonates. From 2,3-dihydro-furan derivs., the displacement of the resulting anomeric xanthate with various nucleophiles in the presence of Lewis acid allowed the formation

of new carbon-carbon and carbon-heteroatom bonds. This strategy was illustrated by a two-step synthesis of a precursor of modified 2'-β-C-branched nucleoside analogs.

IT ***883857-58-7P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 2,3-trans di-substituted tetrahydrofurans as intermediates for 2'-β-C-branched nucleosides through sequential xanthate radical addition-substitution reactions)

RN 883857-58-7 CAPLUS

CN Butanoic acid, 4-butoxy-4-[(ethoxythioxomethyl)thio]-2-fluoro-, ethyl ester (9CI) (CA INDEX NAME)



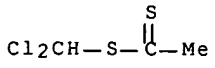
REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:891202 CAPLUS Full-text
DOCUMENT NUMBER: 143:406205
TITLE: Comparison of Bond Dissociation Energies of Dormant Species Relevant to Degenerative Transfer and Atom Transfer Radical Polymerization
AUTHOR(S): Matyjaszewski, Krzysztof; Poli, Rinaldo
CORPORATE SOURCE: Department of Chemistry, Carnegie Mellon University, Pittsburgh, PA, 15213, USA
SOURCE: Macromolecules (2005), 38(19), 8093-8100
CODEN: MAMOBX; ISSN: 0024-9297
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

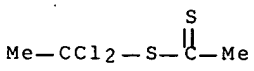
AB D. functional calcns. are reported for the bond dissociation energy (BDE) of a number of dithioacetates, CH3C(S)S-R and selected dithiobenzoates, PhC(S)S-R, of relevance to reversible addition-fragmentation transfer (RAFT) controlled radical polymerization In comparison with previously reported calcns. [Gillies, M. B.; Matyjaszewski, K.; Norrby, P.-O.; Pintauer, T.; Poli, P.; Richard, R. Macromols. 2003, 36, 8551-8559] at the same level on corresponding R-X systems (X = Cl, Br, I, N3, S2CNMe2), the results reveal significant steric and polar effects on the BDE. Particularly bulky R groups (tBu, C(CH3)2COOMe) yield relatively weaker R-S2CZ (Z = Me, Ph) bonds, such that the radical transfer process to R'-S2CZ where R' is less sterically encumbering (e.g., CH(CH3)COOMe) is less favorable, when compared to the same transfer to R'-Cl (or R'-Br). As indicated by an anal. of DFT computed natural charges, electroneg. substituents in the α position of the R group (F, OMe, OAc, and also multiple substitution with Cl atoms) reinforce the ionic component of the R-X bond when X is a more electroneg. group (i.e., Cl, Br) relative to S2CZ. Therefore, transfer of these radicals is also disfavored for R'-S2CZ relative to R'-Cl or R'-Br. These effects rationalize exptl. observations and can be used as a guiding tool for the rational design of ATRP initiators and RAFT transfer agents.

IT ***867212-97-3 867213-00-1***
RL: PRP (Properties)
(d. functional calcns. of bond dissociation energies of dithiobenzoate and dithioacetates as dormant species relevant to degenerative transfer and

atom transfer radical polymerization)
RN 867212-97-3 CAPLUS
CN Ethane(dithioic) acid, dichloromethyl ester (9CI) (CA INDEX NAME)

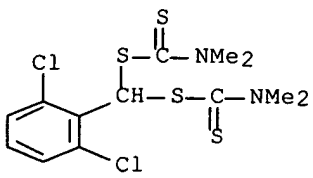


RN 867213-00-1 CAPLUS
CN Ethane(dithioic) acid, 1,1-dichloroethyl ester (9CI) (CA INDEX NAME)

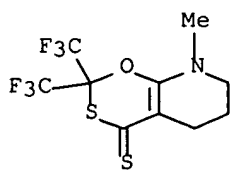


REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1973:505111 CAPLUS Full-text
DOCUMENT NUMBER: 79:105111
TITLE: Synthesis of 2-dialkylamino-1,3-dithietan-2-ylium salt. Action of strong acids on benzylidenebis(N,N-dialkyldithiocarbamates)
AUTHOR(S): Ueno, Yoshio; Okawara, Makoto
CORPORATE SOURCE: Res. Lab. Resour. Util., Tokyo Inst. Technol., Tokyo, Japan
SOURCE: Chemistry Letters (1973), (8), 863-6
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 79:105111
GI For diagram(s), see printed CA Issue.
AB 1,3-Dithietan-2-ylium salts I (R = Me, Et; R1 = H, Cl; X = iodo, ClO4) and II were prepared by protonation of benzylidenebis(dialkyldithiocarbamates), 2,6-R12C6H3CH(S2CNR2)2, with 70% HClO4 or concentrated H2SO4.
IT ***6842-59-7***
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acids)
RN 6842-59-7 CAPLUS
CN Carbamodithioic acid, dimethyl-, (2,6-dichlorophenyl)methylene ester (9CI) (CA INDEX NAME)



L35 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1967:421876 CAPLUS Full-text
DOCUMENT NUMBER: 67:21876
TITLE: Stable 1,4-dipoles from ketene acetals and carbon disulfide and their use for synthesis of heterocycles
AUTHOR(S): Gompper, Rudolf; Elser, Wolfgang
CORPORATE SOURCE: Univ. Munich, Munich, Fed. Rep. Ger.
SOURCE: Angewandte Chemie, International Edition in English (1967), 6(4), 366-7
CODEN: ACIEAY; ISSN: 0570-0833
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 67:21876
GI For diagram(s), see printed CA Issue.
AB The 1,4-dipoles, MeS(Me2N)C+CH2CS2-, (Me2N)2C+CH(R)CS2-, 1-methyl-2-methylthiopyrrolidine-3-dithiocarboxylate dipole (I), and 1-methyl-2-methylthiopiperidine-3-dithiocarboxylate dipole (II), are prepared and treated with ketones and ketenes to give pyridothioxanes, pyridothiins, and pyridothiazines. Also prepared is 5H-1,7-dimethyl- 1,2,3,4,7,8,9,10-octahydrodipyrido[3,2-c:3',2'-e]thiopyran-5-thione (III). Compds. of the general formula RCH:C(SMe)NR12 and ketene aminals are treated with CS2 in MeCN at -40° to give I, II, (Me2N)2C+CH2CS2-, (Me2N)2C+CHMeCS2-, and MeS(Me2N)C+CH2CS2-. II is treated with MeI to give Me 1-methyl-2-methylthiopiperidine-3-dithiocarboxylate iodide, m. 143-5°. II is treated with PhNCO to give 5-methyl-4-phenyl-5,6,7,8- tetrahydro-1H,3H-pyrido[2,3-d]-1,3-thiazine-1,3-dione, m. 197-9°. Also prepared are (m.p. given): 5-methyl-4-phenyl-5,6,7,8-tetrahydro-1H,3H- pyrido[2,3-d]-1,3-thiazine-1-thione-3-one, 194°; 5-methyl-4-phenyl-3-phenylimino-5,6,7,8-tetrahydro-1H,3H-pyrido[2,3-d]-1,3- thiazine-1-thione, 191-3°; 3-diphenylmethylene-5-methyl-5,6,7,8-tetrahydro-1H,3H-pyrido[3,2-e]-4H-1,3-oxathiin-1-thione (IV), 210-11°; 3-(carbomethoxycyanomethylene)-5-methyl-5,6,7,8-tetrahydro- 1H,3H-pyrido[2,3-e]-4H-1,3-oxathiin-1-thione (IV), 223°; 3,3-bis(trifluoromethyl)-5-methyl-5,6,7,8-tetrahydro-1H,3H-pyrido[3,2-e]- 4H-1,3-oxathiin-1-thione, 133°; III, 182-3°; 4-methyl-4,5,6,7-tetrahydro-1H-pyrido[2,3-c]-1,2-dithiole-1-thione, 143-4°; S-diphenylacetyl 1-methyl-2-methylthio-1,4,5,6- tetrahydropyridine-3-dithiocarboxylate (V), 88° (decomposition). I is treated with Ph2C:C:O to give a mixture containing 3-diphenylmethylene-4-methyl- 6,7-dihydro-1H,3H,5H-pyrrolo[3,2-e]-2H,4H-1,3-oxathiin-1-thione, m. 202-3°, and 5-methyl-4,4-diphenyl-3,4,6,7-tetrahydro-1H,5H- pyrrolo[3,2-c]-2H-thiopyran-1-thione-3-one, m. 262-5°. V is kept in a solution in MeCN to give IV. Cycloaddn. to I, II, (Me2N)2C+CHRCS2-, and MeS(Me2N)C+CH2CS2- can occur in 2 stages.
IT ***16151-57-8P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 16151-57-8 CAPLUS
CN 4H-1,3-Oxathiino[6,5-b]pyridine-4-thione, 5,6,7,8-tetrahydro-8-methyl-2,2-bis(trifluoromethyl)- (8CI) (CA INDEX NAME)



L35 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:494051 CAPLUS Full-text
DOCUMENT NUMBER: 65:94051
ORIGINAL REFERENCE NO.: 65:17623b
TITLE: Herbicides
INVENTOR(S): Gradsten, Marcel A.
PATENT ASSIGNEE(S): Tenneco Chemicals, Inc.
SOURCE: 2 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

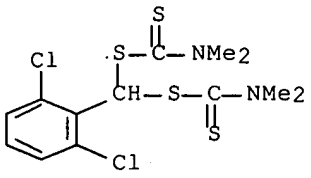
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3266882		19660816	US 1965-488783	19650920

AB A post-emergence spray of 10 lb./acre of (2,6- dichlorophenyl)methylene bis(dimethyldithiocarbamate) (I) gives effective control of crabgrass, foxtail, Johnson grass, mustard, red clover, and morning glory. I, m. 225.5 to 227.5° is made in 30% yield by refluxing 76 g. of 2,6-dichlorobenzal chloride and 110 g. of Me2NCSSNa in 50 ml. of EtOH for 5.5 hrs.

IT ***6842-59-7***, Toluene-α,α-dithiol, 2,6-dichloro-, bis(dimethyldithiocarbamate)
(as herbicide)

RN 6842-59-7 CAPLUS

CN Carbamodithioic acid, dimethyl-, (2,6-dichlorophenyl)methylene ester (9CI) (CA INDEX NAME)



L35 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:494050 CAPLUS Full-text
DOCUMENT NUMBER: 65:94050
ORIGINAL REFERENCE NO.: 65:17622h,17623a-b
TITLE: Herbicidal mixtures
PATENT ASSIGNEE(S): Quinoleine et ses Derives.
SOURCE: 7 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

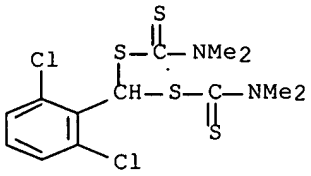
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1432727		19660325	FR 1965-5059	19650210

AB Mixts. of 1 part 4-amino-3,5,6-trichloropicolinic acid (I) and 1-10 parts 2-methoxy-3,6-dichlorobenzoic acid (II), or mixts, of I 1 part and II 3-6 parts with 1-20 parts of one or more phenoxy acid type herbicides, the acids being in the form of metal, alkylamine, or alkanolamine salts or esters, are valuable for the removal of weeds that are resistant to the phenoxy acid herbicides while being harmless to cereal crops. Thus, expts. were carried out using a logarithmic sprayer applying 600 l./ha. to winter and to spring wheat containing Matricaria chamomilla, Stellaria media, Veronica, Polygonum, and Galium aparine. All of the following mixts. gave 80-100% weed kill without damage to the crop: II 120 and MCPA 1440; I 45 and MCPA 540; I 35, II 70, and MCPA 945; and these mixts. of I, II, and MCPA (all in g./ha.) 30, 60, 1080; 25, 75,900; 23, 92,690; 20, 80,900; 18, 108, 756; 15, 90, 945. In a similar experiment with winter wheat, a 25, 75, 700 g./ha. mixture gave best results. The expts. above used the acids as solution of mixed Na and K salts; others used them as butoxyethyl esters. In some expts. mixts. were found that were especially useful for control of one or more difficult species; others were found that caused slight crop damage.

IT ***6842-59-7***, Carbamic acid, dimethyldithio-, 2,6-dichlorobenzylidene ester
(as herbicide)

RN 6842-59-7 CAPLUS

CN Carbamodithioic acid, dimethyl-, (2,6-dichlorophenyl)methylene ester (9CI) (CA INDEX NAME)



L35 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:438317 CAPLUS Full-text

DOCUMENT NUMBER: 65:38317

ORIGINAL REFERENCE NO.: 65:7104e-f

TITLE: 2,6 - Dichlorophenylmethylene bis(N,N - dimethyldithiocarbamate)

INVENTOR(S): Gradsten, Marcel A.

PATENT ASSIGNEE(S): Tenneco Chemicals, Inc.

SOURCE: 2 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

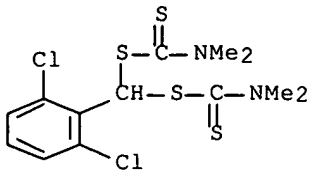
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3257441		19660621	US 1962-179461	19620313
PRIORITY APPLN. INFO.:			US	19620313

AB A mixture of 110 g. NaSC(:S)NMe2, 76 g. 2,6-Cl2C6H3CHCl2, and 150 ml. EtOH was refluxed 5.5 hrs., cooled, filtered, and the filtrate concentrated to give 47 g. 2,6-Cl2C6H3CH[S(S:)CNMe2]2, m. 225.5-7.5°, which is useful as a herbicide.

IT ***6842-59-7P***, Carbamic acid, dimethyldithio-, 2,6-dichlorobenzylidene ester

RL: PREP (Preparation)
(preparation of)
RN 6842-59-7 CAPLUS
CN Carbamodithioic acid, dimethyl-, (2,6-dichlorophenyl)methylene ester (9CI)
(CA INDEX NAME)

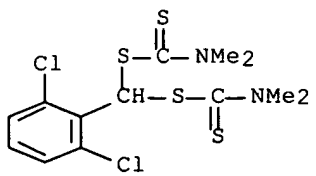


L35 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:438316 CAPLUS Full-text
DOCUMENT NUMBER: 65:38316
ORIGINAL REFERENCE NO.: 65:7104c-e
TITLE: α,α'-Bis(laurylthio)-p-xylene
INVENTOR(S): Braus, Harry; Wass, Fred D.
PATENT ASSIGNEE(S): National Distillers and Chemical Corp.
SOURCE: 2 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3258493		19660628	US	19620911
PRIORITY APPLN. INFO.:			US	19620911

AB The title compds. were prepared by the reaction of ortho, meta, or para dihalide with a Na alkyl sulfide. To a stirred solution of 11.5 g. Na in 200 ml. anhydrous EtOH, 101.2 g. C12H25SH was added slowly, the mixture kept below the b.p., and treated with 43.6 g. p-C6H4(CH2Cl)2 during 1 hr. The solution was refluxed 0.5 hr., washed with hot H2O to remove acl. and NaCl, and evaporated to give 104.3 g. α,α'-bis(laurylthio)-p-xylene (I). I improves resistance to thermal and oxidative degradation in polymers.

IT ***6842-59-7P***, Carbamic acid, dimethyldithio-, 2,6-dichlorobenzylidene ester
RL: PREP (Preparation)
(preparation of)
RN 6842-59-7 CAPLUS
CN Carbamodithioic acid, dimethyl-, (2,6-dichlorophenyl)methylene ester (9CI)
(CA INDEX NAME)



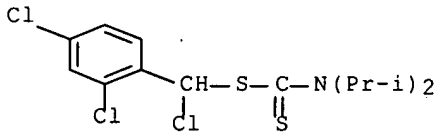
L35 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1965:11837 CAPLUS Full-text
DOCUMENT NUMBER: 62:11837
ORIGINAL REFERENCE NO.: 62:2189h,2190a
TITLE: Phytotoxicity of herbicides as measured by root absorption
AUTHOR(S): Hilton, H. W.; Nomura, N.
CORPORATE SOURCE: Hawaiian Sugar Planters Assoc., Honolulu
SOURCE: Weed Research (1964), 4(3), 216-22
CODEN: WEREAT; ISSN: 0043-1737
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The min. lethal concentration of 7 ureas, 21 s-triazines, 2 uracils, 5 anilides, 7 auxins, 6 carbamates, and 11 other compds. for cucumber, sorghum, and wheat plants was determined None of the compds. was lethal at 10-7M, the most active compound being desmetryne (4-isopropylamino-6-methylamino-2-methylthio-1,3,5-triazine) which was lethal to cucumber at 10-6.85M. Paraquat was the only compound toxic to all 3 species at <10-6M. The triazine derivs. in general showed considerable selectivity to sorghum.

IT ***2877-17-0P***, α-Toluenethiol, α,2,4-trichloro-, diisopropyldithiocarbamate
RL: PREP (Preparation)
(crop response to, min. lethal concns. in)

RN 2877-17-0 CAPLUS

CN Carbamic acid, diisopropyldithio-, α,2,4-trichlorobenzyl ester (7CI, 8CI) (CA INDEX NAME)



L35 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:26595 CAPLUS Full-text
DOCUMENT NUMBER: 60:26595
ORIGINAL REFERENCE NO.: 60:4720a-d
TITLE: N - [2 - (N - Methyldithiocarbamoyl) - 2,2 - dichloroacetyl]-thiourea fungicides
INVENTOR(S): Nagasawa, Masao; Yamamoto, Fukutaro; Takahashi, Yoshiro
PATENT ASSIGNEE(S): Ihara Agricultural Chemical Co.
SOURCE: 6 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 38008997	B4	19630613	JP	19610519

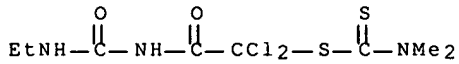
PRIORITY APPLN. INFO.: JP 19610519

AB Compds. of the general formula RR1NCS2CCl2CONHCXNR2R3 (I) were prepared from RR1INCS2Na and Cl3CCONHCXNR2R3. The fungicide effects were examined by the agar dilution streak method against Piricularia oryzae, Xanthomonas pruni, and X. oryzae. The names of the compds. prepared and min. effective concentration (γ/cc.) for the organisms were: N-[2-(N-methyldithiocarbamoyl)-2,2-dichloroacetyl]thiourea, 1, 10, 10; N'[2-(N-methyldithiocarbamoyl)-2,2-dichloroacetyl]-N-phenyl-N-ethylthiourea, 1, 10, 100; N-[2-(N,N-dimethyldithiocarbamoyl)-2,2-dichloro-acetyl] thiourea, 1, 1, 1; N'-[2-(N,N-dimethyldithiocarbamoyl)2,2-dichloroacetyl]-N-phenylthiourea, 1, 1, 10; N'-[2-(N,N-diethyldithiocarbamoyl)-2,2-dichloroacetyl]-N-phenyl- N-ethylthiourea, 1, 10, 100; N-[2-(N-methyldithiocarbamoyl)-2,2- dichloroacetyl]urea, 1, 10, 10; N'-[2-(N-methyldithiocarbamoyl)2,2- dichloroacetyl]-N-phenyl-N-methylurea, 1, 10, 10; N-[2- (N',N-dimethyldithiocarbamoyl)-2,2-dichloroacetyl]urea, 1, 1, 1; N'-[2-(N,N-dimethyldithiocarbamoyl)-2,2-dichloroacetyl]N-ethylurea, 1, 1, 10; N'-[2-(N-ethyldithiocarbamoyl)-2,2dichloroacetyll-N-phenyl-N- methylurea, 1, 10, 100; N-[2(N,N-diethyldithiocarbamoyl)-2,2- dichloroacetyl]urea, 1, 10, 10; control (Dithane), 1, 1, 100. The L.D.90 (γ/cc.) for P. oryzae by the petri dish method were: N-[2-(N,N-dimethyldithiocarbamoyl)-2,2-dichloroacetyllthioura, 0.76; N-[2-(N,N-dimethyldithiocarbamoyl)-2,2-dichloroacetyl]urea, 0.86; Dithane, 0.72 γ/cc.

IT ***90090-18-9P***, Urea, 1-(dichloromercaptoacetyl)-3-ethyl-, dimethyldithiocarbamate ***91394-10-4P***, Urea, 1-(dichloromercaptoacetyl)-3-phenyl-2-thio-, dimethyldithiocarbamate
RL: PREP (Preparation)
(preparation and fungicidal action of)

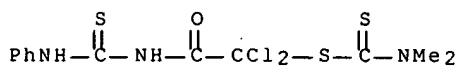
RN 90090-18-9 CAPLUS

CN Carbamic acid, dimethyldithio-, ester with 1-(dichloromercaptoacetyl)-3-ethylurea (7CI) (CA INDEX NAME)



RN 91394-10-4 CAPLUS

CN Carbamic acid, dimethyldithio-, ester with 1-(dichloromercaptoacetyl)-3-phenyl-2-thiourea (7CI) (CA INDEX NAME)



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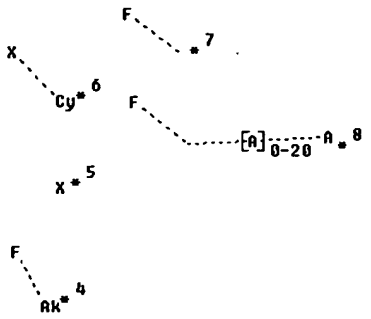

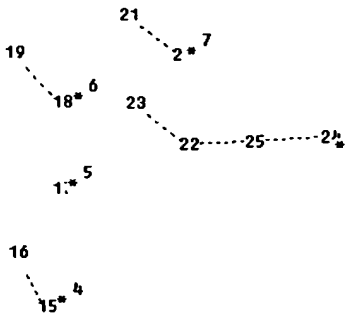

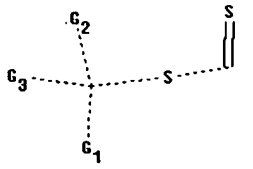

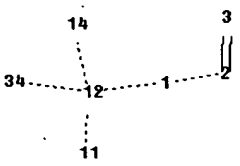

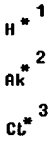

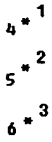

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ring/chain bonds :
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exact/norm bonds :
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G1:[*1],[*2],[*3]

G2:O,S,Cl,Br,I,As,Sb,Se,Te

G3:[*4],[*5],[*6],[*7],[*8]

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:Atom 11:CLASS 12:CLASS 14:CLASS
15:CLASS 16:CLASS 17:CLASS 18:Atom 19:CLASS 20:CLASS 21:CLASS 22:CLASS
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L37            4 SEA FILE=CAOLD ABB=ON  PLU=ON  L12


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                 ANSWERS '13-16' FROM FILE CAOLD

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L38  ANSWER 13 OF 16  CAOLD  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:  CA65:17623b  CAOLD
TITLE:             herbicides
AUTHOR NAME:       Gradsten, Marcel A.
PATENT ASSIGNEE:   Tenneco Chemicals, Inc.
DOCUMENT TYPE:     Patent
     PATENT NO.    KIND         DATE
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PI   US 3266882                 1966
INDEX TERM:          6842-59-7
IT    6842-59-7
RN   6842-59-7  CAOLD
CN   Carbamodithioic acid, dimethyl-, (2,6-dichlorophenyl)methylene ester (9CI)
     (CA INDEX NAME)
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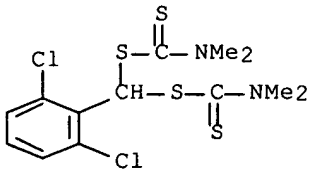


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L38  ANSWER 14 OF 16  CAOLD  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:  CA65:7104e  CAOLD
TITLE:             2,6-dichlorophenylmethylene
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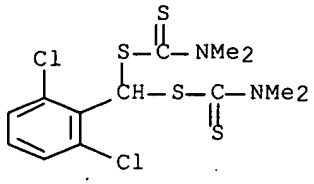
AUTHOR NAME: Gradsten, Marcel A.
DOCUMENT TYPE: Patent
TITLE: 2,6-dichlorophenylmethylene bis(dialkyldithiocarbamates)
PATENT ASSIGNEE: Tenneco Chemicals, Inc.
DOCUMENT TYPE: Patent

PATENT NO.	KIND	DATE
US 3257441		1966

INDEX TERM: ***6842-59-7***
IT ***6842-59-7***
RN 6842-59-7 CAOLD
CN Carbamodithioic acid, dimethyl-, (2,6-dichlorophenyl)methylene ester (9CI) (CA INDEX NAME)



L38 ANSWER 15 OF 16 CAOLD COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: CA62:2189h CAOLD
TITLE: herbicidal control of dwarf mistletoe on California conifers
AUTHOR NAME: Quick, Clarence R.
TITLE: phytotoxicity of herbicides as measured by root absorption
AUTHOR NAME: Hilton, H. Wayne; Nomura, N.
INDEX TERM:

50-31-7	85-34-7	95-06-7	101-42-8	
122-34-9	129-67-9	139-40-2	314-40-9	314-42-1
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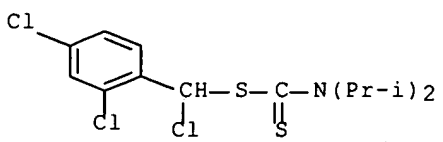
3035-45-8	3084-58-0	31393-14-3		

IT ***2877-17-0***
RN 2877-17-0 CAOLD
CN Carbamic acid, diisopropyldithio-, α,2,4-trichlorobenzyl ester (7CI, 8CI) (CA INDEX NAME)



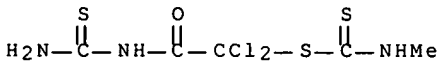
L38 ANSWER 16 OF 16 CAOLD COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: CA60:4720a CAOLD
TITLE: N-[2-(N'-monomethyldithiocarbamoyl)-2,2-dichloroacetyl]thiourea fungicides
AUTHOR NAME: Nagasawa, Masao; Yamamoto, F.; Takahashi, Y.
DOCUMENT TYPE: Patent
TITLE: N-[2-N'-monomethyldithiocarbamoyl)-2,2-dichloracetyl]thiourea fungicides
PATENT ASSIGNEE: Ihara Chemicals Co., Ltd.
DOCUMENT TYPE: Patent

PATENT NO.	KIND	DATE
PI JP 63008997,		1963

INDEX TERM: *89323-68-2* *89463-82-1* *89641-90-7* *90090-17-8* *90090-18-9* *91297-64-2* *91394-10-4* *91394-11-5* *92021-74-4* *92021-76-6* *93089-40-8*

IT *89323-68-2* *89463-82-1* *89641-90-7* *90090-17-8* *90090-18-9* *91297-64-2* *91394-10-4* *91394-11-5* *92021-74-4* *92021-76-6* *93089-40-8*

RN 89323-68-2 CAOLD
CN Carbamic acid, methyldithio-, ester with 1-(dichloromercaptoacetyl)-2-thiourea (7CI) (CA INDEX NAME)



RN 89463-82-1 CAOLD
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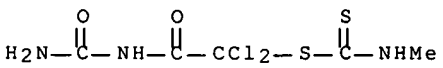

RN 89641-90-7 CAOLD
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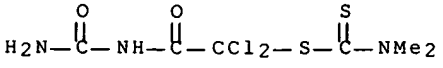
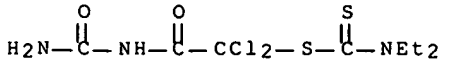
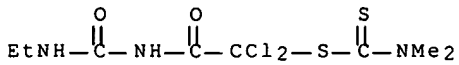


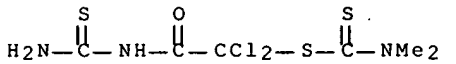
RN 90090-17-8 CAOLD
CN Carbamic acid, diethyldithio-, ester with (dichloromercaptoacetyl)urea (7CI) (CA INDEX NAME)



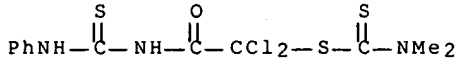
RN 90090-18-9 CAOLD
CN Carbamic acid, dimethyldithio-, ester with 1-(dichloromercaptoacetyl)-3-ethylurea (7CI) (CA INDEX NAME)



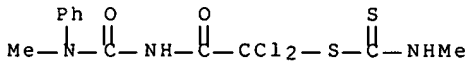
RN 91297-64-2 CAOLD
CN Carbamic acid, dimethyldithio-, ester with 1-(dichloromercaptoacetyl)-2-thiourea (7CI) (CA INDEX NAME)



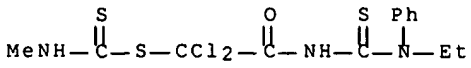
RN 91394-10-4 CAOLD
CN Carbamic acid, dimethyldithio-, ester with 1-(dichloromercaptoacetyl)-3-phenyl-2-thiourea (7CI) (CA INDEX NAME)



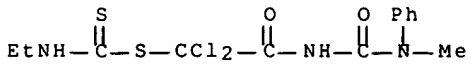
RN 91394-11-5 CAOLD
CN Carbamic acid, methyldithio-, ester with 3-(dichloromercaptoacetyl)methyl-1-phenylurea (7CI) (CA INDEX NAME)



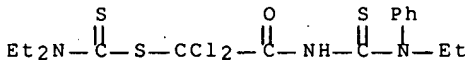
RN 92021-74-4 CAOLD
CN Carbamic acid, methyldithio-, ester with 3-(dichloromercaptoacetyl)-1-ethyl-1-phenyl-2-thiourea (7CI) (CA INDEX NAME)



RN 92021-76-6 CAOLD
CN Carbamic acid, ethyldithio-, ester with 3-(dichloromercaptoacetyl)-1-methyl-1-phenylurea (7CI) (CA INDEX NAME)



RN 93089-40-8 CAOLD
CN Carbamic acid, diethyldithio-, ester with 3-(dichloromercaptoacetyl)-1-ethyl-1-phenyl-2-thiourea (7CI) (CA INDEX NAME)



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=> d his full

     (FILE 'HOME' ENTERED AT 16:33:23 ON 11 APR 2007)

     FILE 'STNGUIDE' ENTERED AT 16:33:46 ON 11 APR 2007

     FILE 'REGISTRY' ENTERED AT 16:34:10 ON 11 APR 2007

     FILE 'CAPLUS' ENTERED AT 16:34:21 ON 11 APR 2007
                E US2005-527702/APPS
L1            1 SEA ABB=ON  PLU=ON  US2005-527702/AP
                D SCA
                SEL RN

     FILE 'REGISTRY' ENTERED AT 16:34:47 ON 11 APR 2007
L2           52 SEA ABB=ON  PLU=ON  (669692-44-8/BI OR 1067-87-4/BI OR
                108-05-4/BI OR 109-49-9/BI OR 109-75-1/BI OR 140-89-6/BI OR
                224425-08-5/BI OR 3054-95-3/BI OR 431-46-9/BI OR 5428-09-1/BI
                OR 583028-99-3/BI OR 583029-00-9/BI OR 583029-01-0/BI OR
                583029-02-1/BI OR 583029-03-2/BI OR 583029-04-3/BI OR 583029-05
                -4/BI OR 583029-07-6/BI OR 583029-08-7/BI OR 583029-09-8/BI OR
                583029-11-2/BI OR 583029-13-4/BI OR 583029-14-5/BI OR 583029-15
                -6/BI OR 583029-16-7/BI OR 591-87-7/BI OR 669692-43-7/BI OR
                669692-45-9/BI OR 669692-46-0/BI OR 669692-47-1/BI OR 669692-48
                -2/BI OR 669692-49-3/BI OR 669692-50-6/BI OR 669692-51-7/BI OR
                669692-52-8/BI OR 669692-53-9/BI OR 669692-54-0/BI OR 669692-55
                -1/BI OR 669692-56-2/BI OR 669692-57-3/BI OR 669692-58-4/BI OR
                669692-59-5/BI OR 669692-60-8/BI OR 669692-61-9/BI OR 669692-64
                -2/BI OR 6776-45-0/BI OR 6776-46-1/BI OR 754-05-2/BI OR
                762-04-9/BI OR 762-72-1/BI OR 872-36-6/BI OR 88-12-0/BI)

     FILE 'CAPLUS' ENTERED AT 16:36:45 ON 11 APR 2007
L3            1 SEA ABB=ON  PLU=ON  L2/P AND L1
                D SCA
                SEL RN

     FILE 'REGISTRY' ENTERED AT 16:37:06 ON 11 APR 2007
L4           52 SEA ABB=ON  PLU=ON  (669692-44-8/BI OR 1067-87-4/BI OR
                108-05-4/BI OR 109-49-9/BI OR 109-75-1/BI OR 140-89-6/BI OR
                224425-08-5/BI OR 3054-95-3/BI OR 431-46-9/BI OR 5428-09-1/BI
                OR 583028-99-3/BI OR 583029-00-9/BI OR 583029-01-0/BI OR
                583029-02-1/BI OR 583029-03-2/BI OR 583029-04-3/BI OR 583029-05
                -4/BI OR 583029-07-6/BI OR 583029-08-7/BI OR 583029-09-8/BI OR
                583029-11-2/BI OR 583029-13-4/BI OR 583029-14-5/BI OR 583029-15
                -6/BI OR 583029-16-7/BI OR 591-87-7/BI OR 669692-43-7/BI OR
                669692-45-9/BI OR 669692-46-0/BI OR 669692-47-1/BI OR 669692-48
                -2/BI OR 669692-49-3/BI OR 669692-50-6/BI OR 669692-51-7/BI OR
                669692-52-8/BI OR 669692-53-9/BI OR 669692-54-0/BI OR 669692-55
                -1/BI OR 669692-56-2/BI OR 669692-57-3/BI OR 669692-58-4/BI OR
                669692-59-5/BI OR 669692-60-8/BI OR 669692-61-9/BI OR 669692-64
                -2/BI OR 6776-45-0/BI OR 6776-46-1/BI OR 754-05-2/BI OR
                762-04-9/BI OR 762-72-1/BI OR 872-36-6/BI OR 88-12-0/BI)

     FILE 'CAPLUS' ENTERED AT 16:37:44 ON 11 APR 2007
                SEL HIT RN L3

     FILE 'REGISTRY' ENTERED AT 16:38:00 ON 11 APR 2007
L5           37 SEA ABB=ON  PLU=ON  (669692-44-8/BI OR 583028-99-3/BI OR
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                583029-00-9/BI OR 583029-01-0/BI OR 583029-02-1/BI OR 583029-03
                -2/BI OR 583029-04-3/BI OR 583029-05-4/BI OR 583029-07-6/BI OR
                583029-08-7/BI OR 583029-09-8/BI OR 583029-11-2/BI OR 583029-13
                -4/BI OR 583029-14-5/BI OR 583029-15-6/BI OR 583029-16-7/BI OR
                669692-43-7/BI OR 669692-45-9/BI OR 669692-46-0/BI OR 669692-47
                -1/BI OR 669692-48-2/BI OR 669692-49-3/BI OR 669692-50-6/BI OR
                669692-51-7/BI OR 669692-52-8/BI OR 669692-53-9/BI OR 669692-54
                -0/BI OR 669692-55-1/BI OR 669692-56-2/BI OR 669692-57-3/BI OR
                669692-58-4/BI OR 669692-59-5/BI OR 669692-60-8/BI OR 669692-61
                -9/BI OR 669692-64-2/BI OR 6776-45-0/BI OR 6776-46-1/BI)
                D SCA
L6              STRUCTURE UPLOADED
L7            2 SEA SSS SAM L6
                D SCA
L8              STRUCTURE UPLOADED
L9            2 SEA SSS SAM L8
L10             STRUCTURE UPLOADED
L11           1 SEA SSS SAM L10
                D SCA
L12          31 SEA SSS FUL L10
                SAVE TEMP NWA702STR10L/A L12
L13           2 SEA ABB=ON  PLU=ON  L7 AND L12
L14           2 SEA ABB=ON  PLU=ON  L9 AND L12

     FILE 'CAPLUS' ENTERED AT 16:50:03 ON 11 APR 2007
L15          22 SEA ABB=ON  PLU=ON  L12

     FILE 'REGISTRY' ENTERED AT 16:50:57 ON 11 APR 2007

     FILE 'BEILSTEIN' ENTERED AT 16:51:04 ON 11 APR 2007
L16           1 SEA SSS SAM L10
L17          20 SEA SSS FUL L10
L18           6 SEA ABB=ON  PLU=ON  L17 AND BABSAN/FA
                SEL BABSAN

     FILE 'BABS' ENTERED AT 16:52:19 ON 11 APR 2007
L19           5 SEA ABB=ON  PLU=ON  (6503908/BABSAN OR 6277633/BABSAN OR
                6409259/BABSAN OR 6540385/BABSAN OR 6565731/BABSAN)

     FILE 'CAPLUS, BABS' ENTERED AT 16:52:53 ON 11 APR 2007
L20          22 DUP REM L15 L19 (5 DUPLICATES REMOVED)
                     ANSWERS '1-22' FROM FILE CAPLUS

     FILE 'REGISTRY' ENTERED AT 16:53:00 ON 11 APR 2007
L21           2 SEA ABB=ON  PLU=ON  L12 AND BEILSTEIN/LC
L22           0 SEA ABB=ON  PLU=ON  L21 NOT CAPLUS/LC

     FILE 'BEILSTEIN' ENTERED AT 16:53:59 ON 11 APR 2007
L23           2 SEA ABB=ON  PLU=ON  L17 AND RN/FA
L24          12 SEA ABB=ON  PLU=ON  L17 NOT (L18 OR L23)
L25           0 SEA ABB=ON  PLU=ON  L24 AND 2005

     FILE 'CAPLUS' ENTERED AT 16:55:41 ON 11 APR 2007

     FILE 'CAPLUS' ENTERED AT 16:58:25 ON 11 APR 2007
L26         274 SEA ABB=ON  PLU=ON  ZARD S?/AU
L27          16 SEA ABB=ON  PLU=ON  GAGOSZ F?/AU
L28          73 SEA ABB=ON  PLU=ON  TOURNIER L?/AU
L29          10 SEA ABB=ON  PLU=ON  L26 AND (L27 OR L28)
L30           0 SEA ABB=ON  PLU=ON  L27 AND L28
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L31          10 SEA ABB=ON  PLU=ON  (L29 OR L30)
L32          10 SEA ABB=ON  PLU=ON  L15 AND (L26 OR L27 OR L28)
L33           4 SEA ABB=ON  PLU=ON  L31 AND L32

     FILE 'BEILSTEIN' ENTERED AT 17:00:24 ON 11 APR 2007

     FILE 'CAPLUS' ENTERED AT 17:01:33 ON 11 APR 2007

     FILE 'REGISTRY' ENTERED AT 17:01:52 ON 11 APR 2007

     FILE 'CAPLUS' ENTERED AT 17:01:54 ON 11 APR 2007
               D STAT QUE L31
               D STAT QUE L32
L34          16 SEA ABB=ON  PLU=ON  (L31 OR L32)
               D IBIB ABS HITSTR L34 1-16

     FILE 'REGISTRY' ENTERED AT 17:02:44 ON 11 APR 2007

     FILE 'CAPLUS' ENTERED AT 17:02:46 ON 11 APR 2007
               D STAT QUE L15
L35          12 SEA ABB=ON  PLU=ON  L15 NOT L34
               D IBIB ABS HITSTR L35 1-12

     FILE 'REGISTRY' ENTERED AT 17:05:42 ON 11 APR 2007
L36            ANALYZE PLU=ON  L12 1- LC :       8 TERMS
               D

     FILE 'CAOLD' ENTERED AT 17:06:15 ON 11 APR 2007
L37           4 SEA ABB=ON  PLU=ON  L12

     FILE 'REGISTRY' ENTERED AT 17:06:49 ON 11 APR 2007

     FILE 'CAOLD' ENTERED AT 17:06:54 ON 11 APR 2007
               D STAT QUE L37

     FILE 'CAPLUS, CAOLD' ENTERED AT 17:07:07 ON 11 APR 2007
L38          16 DUP REM L35 L37 (0 DUPLICATES REMOVED)
                      ANSWERS '1-12' FROM FILE CAPLUS
                      ANSWERS '13-16' FROM FILE CAOLD
               D IALL HITSTR L38 13-16


     FILE HOME

     FILE STNGUIDE
     FILE CONTAINS CURRENT INFORMATION.
     LAST RELOADED: Apr  6, 2007 (20070406/UP).

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:   10 APR 2007  HIGHEST RN 929680-66-0
     DICTIONARY FILE UPDATES:  10 APR 2007  HIGHEST RN 929680-66-0

     New CAS Information Use Policies, enter HELP USAGETERMS for details.

     TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

       Please note that search-term pricing does apply when
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conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

FILE CAPLUS

FILE COVERS 1907 - 11 Apr 2007 VOL 146 ISS 16
FILE LAST UPDATED: 10 Apr 2007 (20070410/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

FILE BEILSTEIN
FILE LAST UPDATED ON JANUARY 10, 2007

FILE COVERS 1771 TO 2006.
FILE CONTAINS 9,780,003 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

****
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *
****

NEW

* ***PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.***
* ***NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES,***

ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

FILE BABS
FILE LAST UPDATED: 10 JAN 2007 <20070110/UP>
FILE COVERS 1980 TO DATE.

FILE CAOLD
FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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